



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2020 – 01:12 PM BST

PDB ID : 6YT7  
Title : GLYCOSYLATED KNOB/DUMMY-HOLE FC FRAGMENT  
Authors : Kuglstatter, A.; Leibrock, L.; Benz, J.  
Deposited on : 2020-04-24  
Resolution : 1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

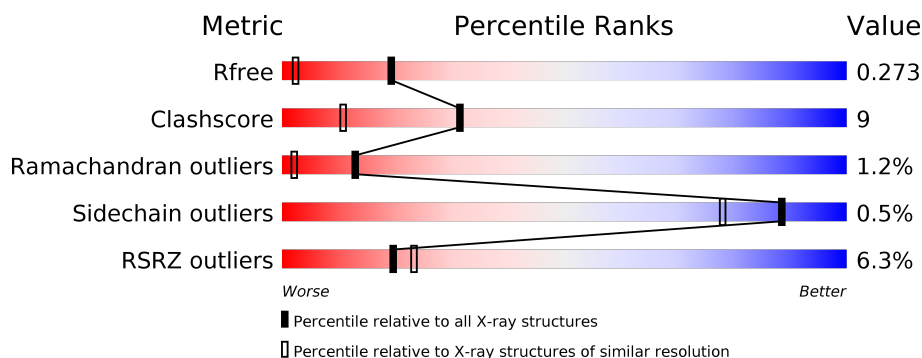
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	232	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>• •</div> <div>8%</div> </div> </div>
3	C	8	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
3	D	8	<div> <div>38%</div> <div>50%</div> <div>13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	7	0
			1718	1097	286	327	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	TRP	THR	engineered mutation	UNP P0DOX5
A	370	GLU	LYS	engineered mutation	UNP P0DOX5
A	448	GLY	-	expression tag	UNP P0DOX5
A	449	GLY	-	expression tag	UNP P0DOX5
A	450	GLY	-	expression tag	UNP P0DOX5
A	451	GLY	-	expression tag	UNP P0DOX5
A	452	SER	-	expression tag	UNP P0DOX5
A	453	HIS	-	expression tag	UNP P0DOX5
A	454	HIS	-	expression tag	UNP P0DOX5
A	455	HIS	-	expression tag	UNP P0DOX5
A	456	HIS	-	expression tag	UNP P0DOX5
A	457	HIS	-	expression tag	UNP P0DOX5
A	458	HIS	-	expression tag	UNP P0DOX5
A	459	HIS	-	expression tag	UNP P0DOX5
A	460	HIS	-	expression tag	UNP P0DOX5

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	8	0
			1720	1096	288	328	8			

There are 4 discrepancies between the modelled and reference sequences:

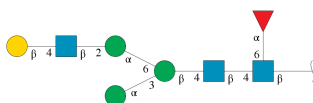
Chain	Residue	Modelled	Actual	Comment	Reference
B	349	CYS	TYR	engineered mutation	UNP P01857

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	366	SER	THR	engineered mutation	UNP P01857
B	368	ALA	LEU	engineered mutation	UNP P01857
B	407	VAL	TYR	engineered mutation	UNP P01857

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			96	54	3	39			
3	D	8	Total	C	N	O	0	0	0
			96	54	3	39			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	120	Total	O	0	0
			120	120		



Chain D:



MA1
MA2
MA3
MA4
MA5
MA6
MA7
MA8

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.02Å 75.10Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.11 – 1.55 74.72 – 1.55	Depositor EDS
% Data completeness (in resolution range)	79.0 (67.11-1.55) 79.1 (74.72-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.55Å)	Xtriage
Refinement program	PHENIX dev_3893	Depositor
R, $R_{free}$	0.234 , 0.273 0.234 , 0.273	Depositor DCC
$R_{free}$ test set	3215 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GAL, BMA, NAG, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	0/1768	1.06	9/2402 (0.4%)
2	B	0.67	2/1772 (0.1%)	1.79	22/2406 (0.9%)
All	All	0.60	2/3540 (0.1%)	1.47	31/4808 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	6
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	416	ARG	CB-CG	-8.17	1.30	1.52
2	B	416	ARG	CG-CD	-5.53	1.38	1.51

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	GLU	OE1-CD-OE2	-42.66	72.11	123.30
2	B	357	GLU	OE1-CD-OE2	-31.71	85.24	123.30
2	B	269	GLU	CG-CD-OE1	23.45	165.21	118.30
1	A	356	ASP	CB-CG-OD1	22.85	138.87	118.30
2	B	443	LEU	CB-CG-CD2	-21.54	74.38	111.00

There are no chirality outliers.



5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	GLU	Sidechain
1	A	356	ASP	Sidechain
2	B	268	HIS	Peptide
2	B	355	ARG	Sidechain
2	B	357	GLU	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1718	0	1670	38	1
2	B	1720	0	1675	20	0
3	C	96	0	82	2	0
3	D	96	0	82	1	1
4	A	85	0	0	9	2
4	B	120	0	0	4	2
All	All	3835	0	3509	58	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:ASN:O	2:B:288:LYS:NZ	1.90	1.03
2:B:347[A]:GLN:OE1	4:B:601:HOH:O	1.89	0.89
1:A:357:GLU:HG2	1:A:360:LYS:HE2	1.55	0.88
1:A:360:LYS:HE3	1:A:362:GLN:O	1.82	0.79
1:A:389:ASN:ND2	4:A:604:HOH:O	2.17	0.78

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:601:HOH:O	4:B:665:HOH:O[3_555]	2.02	0.18
1:A:384:ASN:ND2	3:D:5:NAG:O3[3_555]	2.13	0.07
4:A:656:HOH:O	4:B:674:HOH:O[1_455]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/245 (83%)	195 (96%)	7 (3%)	1 (0%)	29	9
2	B	204/232 (88%)	197 (97%)	3 (2%)	4 (2%)	7	1
All	All	407/477 (85%)	392 (96%)	10 (2%)	5 (1%)	13	2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ASP
2	B	269	GLU
2	B	419	GLN
2	B	361	ASN
2	B	296	TYR

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/223 (90%)	200 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	201/214 (94%)	199 (99%)	2 (1%)	76	57
All	All	401/437 (92%)	399 (100%)	2 (0%)	88	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	355	ARG
2	B	370[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	389	ASN
1	A	421	ASN
2	B	419	GLN
2	B	421	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1	1,3	14,14,15	0.52	0	17,19,21	0.76	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
3	BMA	C	3	3	11,11,12	0.98	1 (9%)	15,15,17	1.17	2 (13%)
3	MAN	C	4	3	11,11,12	1.05	0	15,15,17	1.51	3 (20%)
3	NAG	C	5	3	14,14,15	0.75	1 (7%)	17,19,21	0.71	0
3	GAL	C	6	3	11,11,12	1.09	1 (9%)	15,15,17	1.30	2 (13%)
3	MAN	C	7	3	11,11,12	1.39	1 (9%)	15,15,17	1.17	2 (13%)
3	FUC	C	8	3	10,10,11	0.63	0	14,14,16	0.71	0
3	NAG	D	1	3,2	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.67	0
3	BMA	D	3	3	11,11,12	0.68	0	15,15,17	0.77	0
3	MAN	D	4	3	11,11,12	1.00	1 (9%)	15,15,17	1.25	2 (13%)
3	NAG	D	5	3	14,14,15	0.49	0	17,19,21	0.60	0
3	GAL	D	6	3	11,11,12	1.25	1 (9%)	15,15,17	1.23	2 (13%)
3	MAN	D	7	3	11,11,12	1.34	1 (9%)	15,15,17	1.03	0
3	FUC	D	8	3	10,10,11	1.26	2 (20%)	14,14,16	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	GAL	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	FUC	C	8	3	-	-	0/1/1/1
3	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	0/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C1-C2	3.06	1.59	1.52
3	C	6	GAL	C1-C2	3.03	1.59	1.52
3	D	6	GAL	C1-C2	3.00	1.59	1.52
3	C	7	MAN	O5-C1	-2.80	1.39	1.43
3	D	7	MAN	O5-C1	-2.73	1.39	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	3.59	117.06	112.19
3	D	4	MAN	O2-C2-C3	-3.51	103.10	110.14
3	C	4	MAN	O2-C2-C3	-3.49	103.16	110.14
3	D	4	MAN	C1-O5-C5	2.60	115.72	112.19
3	D	6	GAL	O3-C3-C4	-2.60	104.34	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

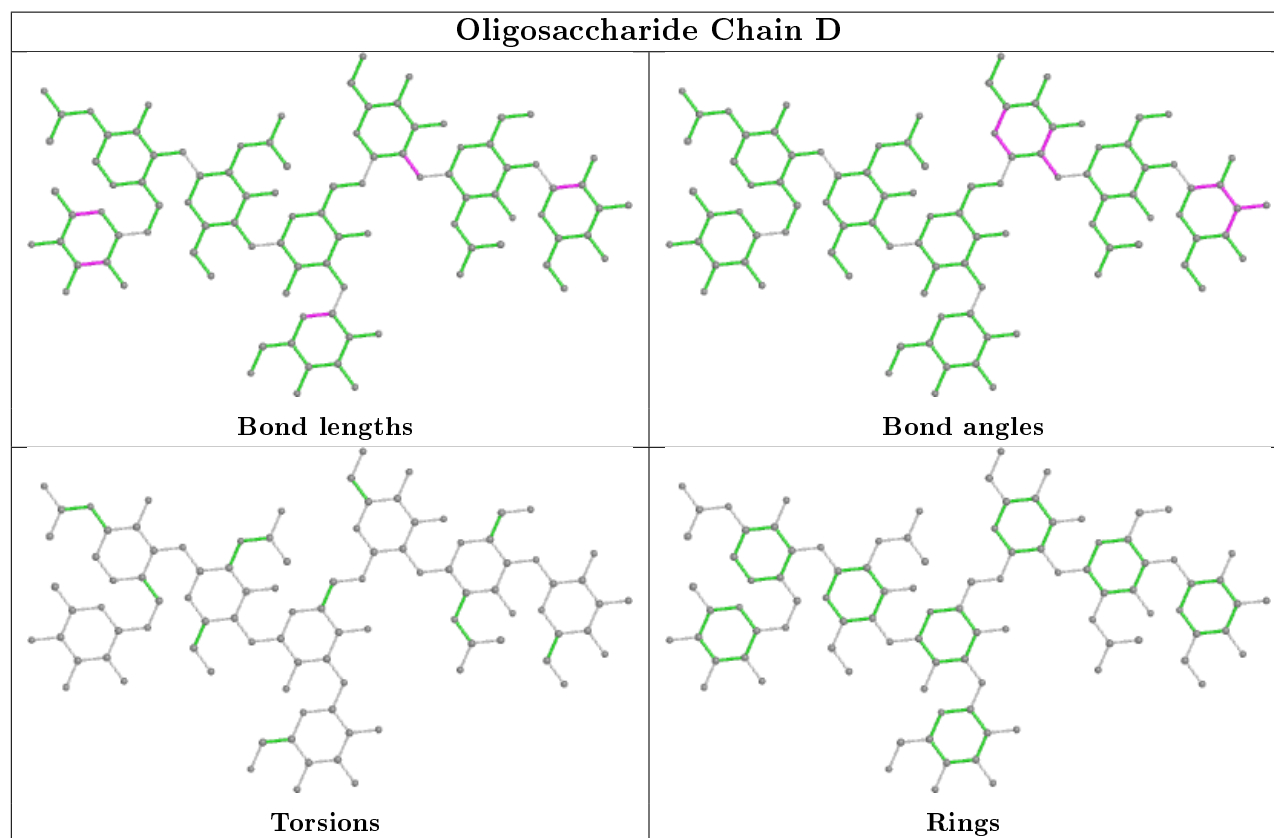
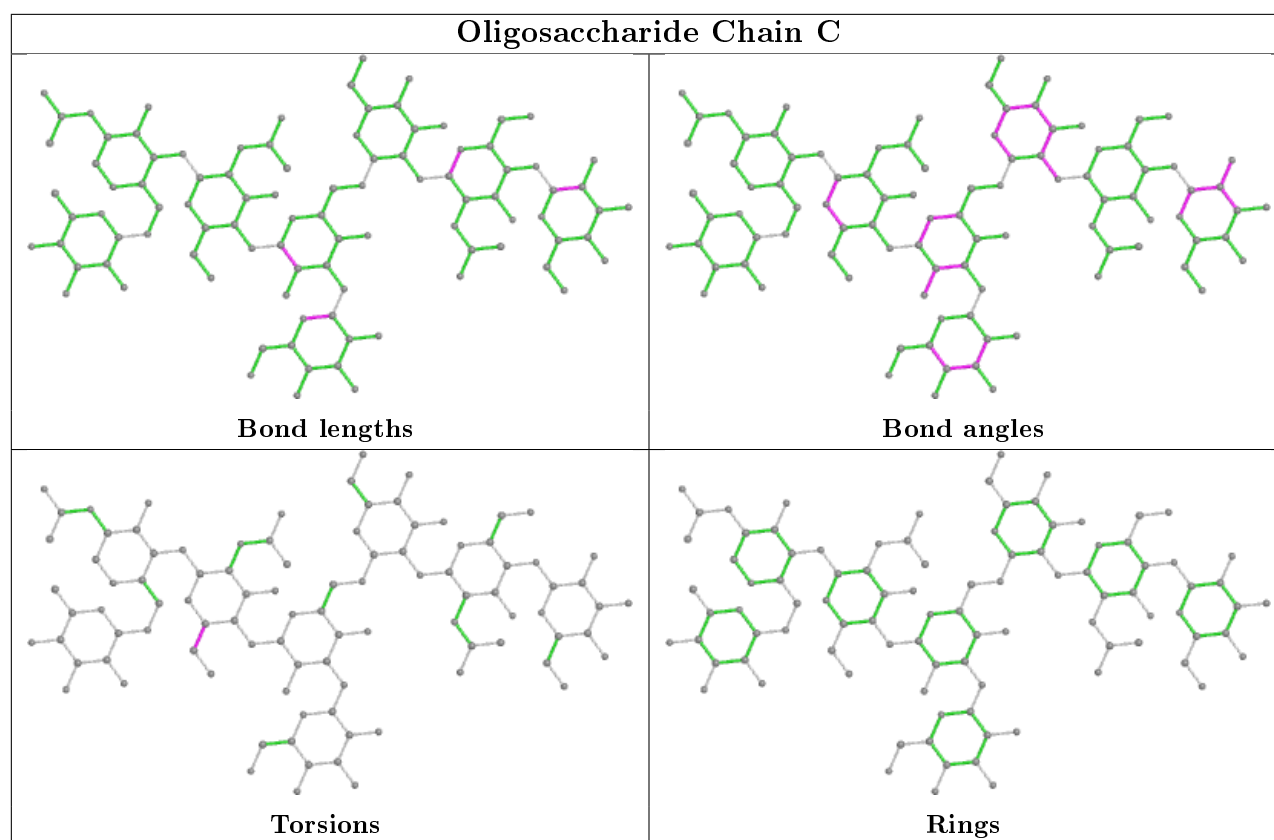
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	NAG	0	1
3	C	5	NAG	1	0
3	D	6	GAL	1	0
3	C	6	GAL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	213/245 (86%)	0.59	17 (7%) 12 14	18, 33, 72, 82	10 (4%)
2	B	213/232 (91%)	0.40	10 (4%) 31 36	17, 31, 53, 81	10 (4%)
All	All	426/477 (89%)	0.50	27 (6%) 20 23	17, 32, 65, 82	20 (4%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	358	LEU	11.3
2	B	355	ARG	5.8
1	A	296	TYR	5.6
1	A	358	LEU	4.6
2	B	359	THR	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	C	7	11/12	0.58	0.18	66,69,72,74	0
3	NAG	C	2	14/15	0.73	0.14	49,55,59,63	0
3	FUC	D	8	10/11	0.75	0.17	39,43,47,49	0
3	FUC	C	8	10/11	0.76	0.26	61,67,70,70	0
3	NAG	C	5	14/15	0.79	0.16	38,42,44,46	0

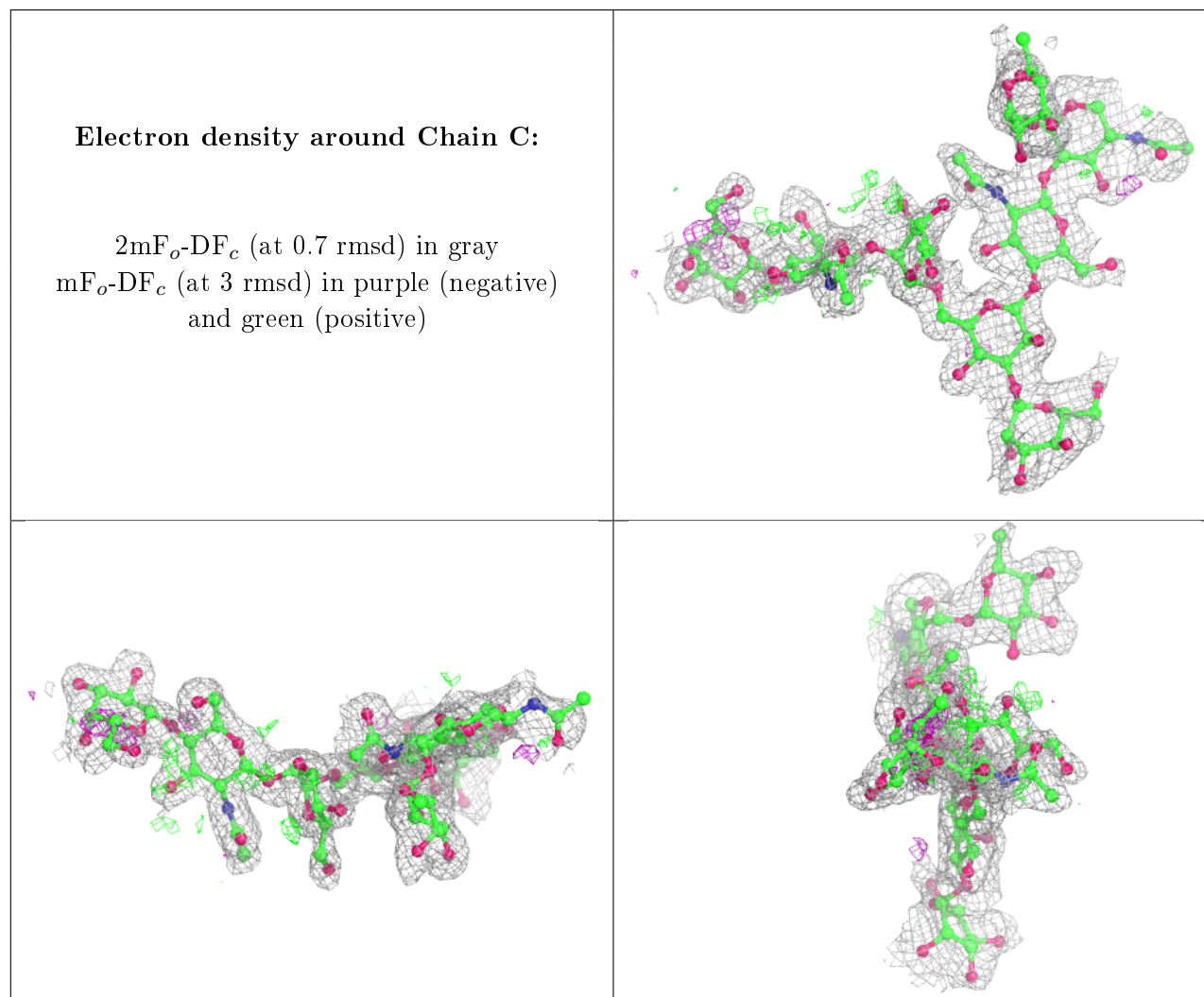
*Continued on next page...*

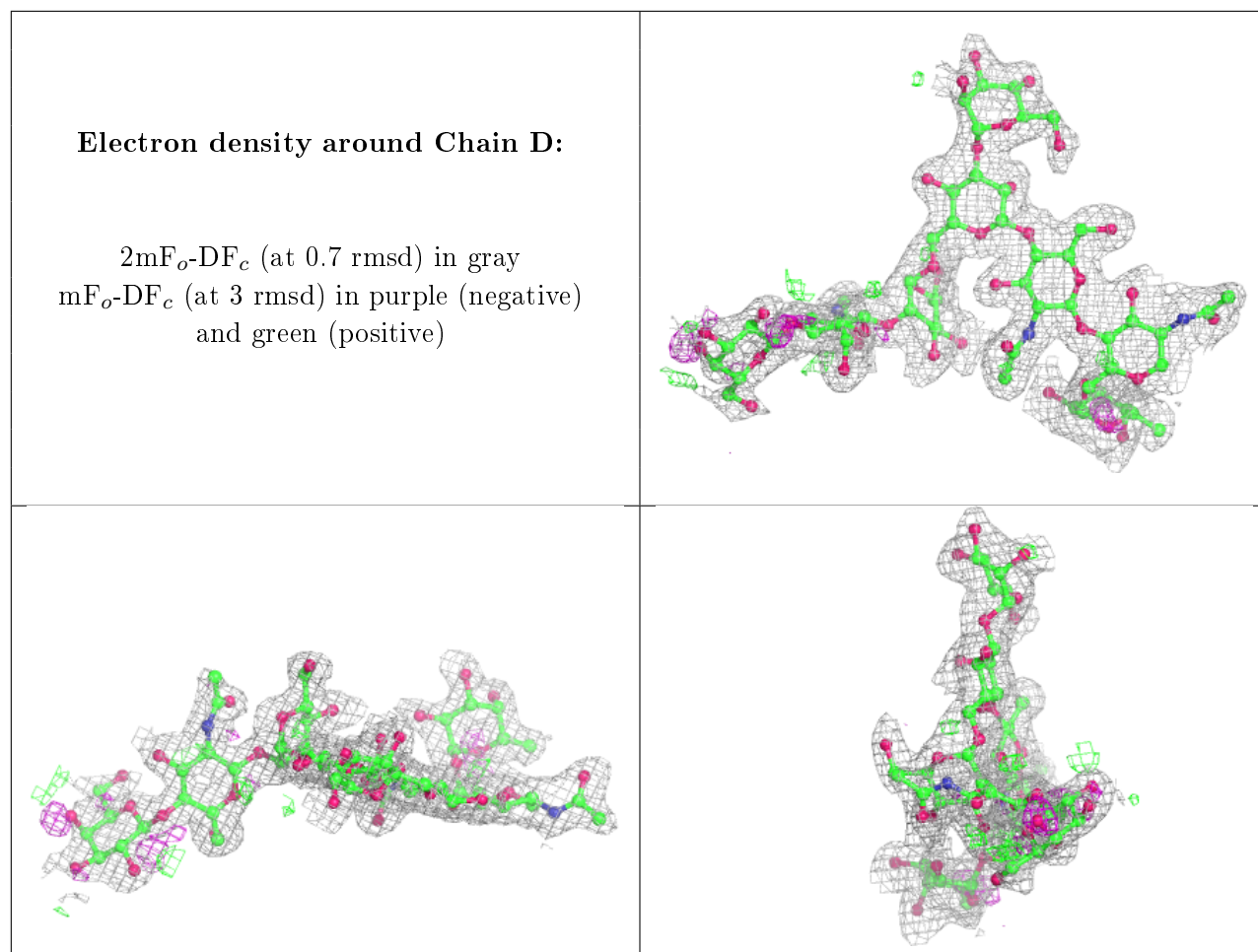


*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	1	14/15	0.79	0.14	61,63,70,73	0
3	NAG	D	5	14/15	0.79	0.15	33,44,48,49	0
3	BMA	C	3	11/12	0.80	0.09	41,46,54,54	0
3	GAL	C	6	11/12	0.81	0.20	34,38,45,46	0
3	GAL	D	6	11/12	0.82	0.25	37,43,56,59	0
3	MAN	D	7	11/12	0.85	0.16	50,57,59,62	0
3	MAN	D	4	11/12	0.86	0.11	33,40,45,46	0
3	MAN	C	4	11/12	0.88	0.15	37,45,50,54	0
3	NAG	D	2	14/15	0.88	0.09	32,39,43,44	0
3	BMA	D	3	11/12	0.89	0.09	36,39,44,44	0
3	NAG	D	1	14/15	0.90	0.08	33,38,45,48	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.